

PARALLELISM OF STABLE TRACES

Jernej Rus

Abelium d.o.o.

Leskoškova cesta 9e, 1000 Ljubljana, Slovenia

jernej.rus@gmail.com

December 28, 2016

Abstract

A d -stable trace is a closed walk which traverses every edge of a graph exactly twice and for every vertex v , there is no subset $N \subseteq N(v)$ ($1 \leq |N| \leq d$), such that every time the walk enters v from N , it also exits to a vertex in N . In addition, in a parallel d -stable trace, every edge is traversed twice in the same direction. d -stable traces were investigated in [Strong traces model of self-assembly polypeptide structures, MATCH Commun. Math. Comput. Chem. **71** (2014), 199–212] as a mathematical model for an innovative biotechnological procedure. It was proven there, that graphs that admit parallel d -stable traces are precisely Eulerian graphs with minimum degree strictly higher than d . In present paper we give an alternative proof of this result by thoroughly examining the special case for $d = 2$. We also explain its importance for synthetic biology and present two algorithms which can be in special cases used for their construction.

Keywords: Eulerian graph; parallel d -stable trace; nanostructure design; self-assembling; polypeptide

AMS Subject Classification (2010): 05C45, 05C85, 94C15

1 Introduction

In 2013 Gradišar et al. [4] presented a novel self-assembly strategy for polypeptide nanostructure design relying on modularization and using orthogonal dimerizing segments. This could lead to significant developments in biotechnology since nanostructures formed by self-assembly of biopolymers and especially polypeptides are known to be one of the most complex in nature. The main success of their research is a construction of a polypeptide self-assembling tetrahedron by concatenating 12 coiled-coil-forming segments separated by flexible peptide hinges in a prescribed order. To be more precise, a single polypeptide chain consisting of 12 segments was routed through 6 edges of the tetrahedron in such a way that every edge was traversed exactly twice. In this way 6 coiled-coil dimers were created and interlocked into a stable tetrahedral structure. This design also provides a foundation for all further investigations about polypeptide folds based constructions using the set of orthogonal interacting polypeptide segments. The required mathematical support for the particular case of the tetrahedron and the general case of polyhedron was already given in [4, 6, 2], where authors explained that polyhedron P that is composed from a single polymer chain can be naturally represented by a graph $G(P)$ of the polyhedron. As every edge of $G(P)$ corresponds to a coiled-coil dimer in the self-assembly process, exactly two biomolecular segments are associated with every edge of $G(P)$. Hence, closed walks that traverse every edge of $G(P)$ precisely twice, called double traces of $G(P)$, play a key role in modeling the construction process. The stability of the constructed polyhedra depends on an additional property whether in the double trace the neighborhoods of vertices can be split.

All graphs considered in this paper will be connected, finite, and simple, that is, without loops and multiple edges. If v is a vertex of a graph G , then its degree will be denoted by $d_G(v)$ or $d(v)$ for short if G will be clear from the context. The *minimum* and the *maximum* degree of G are denoted with $\delta(G)$ and $\Delta(G)$, respectively. A *directed graph* is a graph, where edges have a direction associated with them. In formal terms a directed graph is a pair $G = (V, A)$, where V is a set of vertices and A is a set of ordered pairs of vertices, called *arcs*. A maximal connected subgraph of G is called a *component* of G , while a vertex, which separates two other vertices of the same component is a *cutvertex*, and an edge separating its ends is a *bridge*. A maximal connected subgraph without a cutvertex is called a *block*. Thus, every block of a graph G is either a maximal 2-connected subgraph, or a bridge (with its ends), or an isolated vertex. For other general terms and concepts from graph theory not recalled here we refer to [9].

A *circuit* is a closed walk allowing repetitions of vertices and edges. A *double trace* in a graph G is a circuit which traverses every edge exactly twice. For a set of vertices $N \subseteq N(v)$, we say that a double trace W has a *N -repetition* at vertex v (nontrivial N -repetition in [2]), if N is nonempty, $N \neq N(v)$, and whenever W comes to v from a vertex in N it also continues to a vertex in N . An N -repetition (at v) is a *d -repetition*

if $|N| = d$ (repetition of *order* d), see Fig. 1. Clearly if W has an N -repetition at v , then it also has an $N(v) \setminus N$ -repetition at v (*symmetry of repetitions*). We call a double trace without nontrivial repetitions of order $\leq d$ a *d-stable trace*. Note, that for every $d' \leq d$, a d -stable trace is also a d' -stable trace.

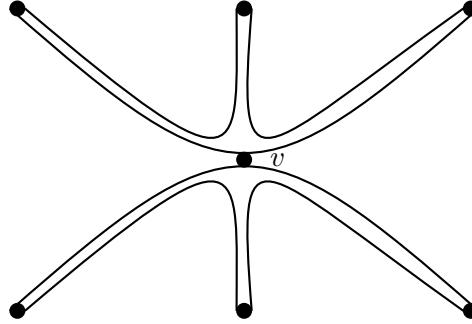


Figure 1: A 3-repetition in a vertex v of degree 6

In order to present a mathematical model for the biotechnological procedure from [4] the graphs that admit d -stable traces were characterized in [2] (thus generalizing results of Sabidussi [7] and Eggleton and Skilton [1] about 1-stable traces and Klavžar and Rus [6] about 2-stable traces) as follows:

Proposition 1.1 [2, Proposition 3.4] *A connected graph G admits a d -stable trace if and only if $\delta(G) > d$.*

Let now W be a double trace of a graph G . Then every edge $e = uv$ of G is traversed exactly twice. If in both cases e is traversed in the same direction (either both times from u to v or both times from v to u) we say that e is a *parallel edge* (with respect to W). If this is not the case we say that e is an *antiparallel edge*. A condition that all the edges of G are of the same type is called a *parallelism*. A double trace W is a *parallel double trace* if every edge of G is parallel and an *antiparallel double trace* if every edge of G is antiparallel. This coincide with chemical properties of peptides. Two peptides may be glued together in such way that they both point in the same direction. In this case they form a parallel dimer. If they point in opposite directions, they form an antiparallel dimer. By now more parallel coiled-coil dimers have been characterized for the molecular design than antiparallel dimers [5]. It is therefore more applicable to investigate parallel double traces.

By replacing every edge of a graph with two new edges we can quickly prove that every graph (every Eulerian graph) admits an antiparallel (parallel) double trace, observation made by several authors, Klavžar and Rus in [6] among others. While graphs admitting antiparallel d -stable traces were characterized in [8], the characterization of

parallel d -stable traces were only mentioned as a consequence in [2]. Therefore, we present an alternative proof of this result in present paper.

We can note right away that parallel double traces do not contain 1-repetitions. Note also that none of the operations that we will use on double traces (concatenations, contractions, deletions, inductive constructions, and reordering) will change the orientation of the edges.

2 Graphs admitting parallel 2-stable traces

The first mathematical model, which was introduced in [6], stated that a polyhedral graph P can be realized by interlocking pairs of polypeptide chains if its corresponding graph $G(P)$ contains a 2-stable trace. Two important deficiencies of this model were later found in [2]: (i) it does not account for vertices of degree ≤ 2 , and (ii) it does not successfully model vertices of degree ≥ 6 (because a polyhedron could split into two parts in a vertex of degree ≥ 6 , as can be seen at Fig. 1 and therefore the structure would not be stable). Since until now, a construction of a polyhedron whose graph of polyhedron would have such properties, has not yet been tried, we first study parallel 2-stable traces in this section.

To make the arguments in this section more transparent, we explain how the reader can graphically imagine 1-repetitions and 2-repetitions in double traces. We can say that a double trace contains an 1-repetition if it has an immediate succession of an edge e by its parallel copy. If v is a vertex of a graph G with a double trace W and u and w are two different neighbors of v , then we can say that W contains a 2-repetition (through) v if the vertex sequence $u \rightarrow v \rightarrow w$ appears twice in W in any direction ($u \rightarrow v \rightarrow w$ or $w \rightarrow v \rightarrow u$), see Fig. 2.

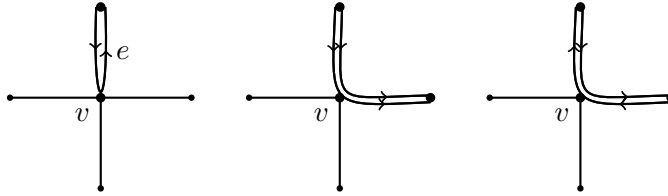


Figure 2: Possible 1- and 2-repetitions of a double trace

We will need the result of next lemma in the proof of Theorem 2.3.

Lemma 2.1 *Let G be a graph and H_1, \dots, H_k its pairwise edge and vertex disjoint subtrees, for $k \geq 0$. Let for every i and for every vertex $v \in V(G) \setminus V(H_i)$, v has at most one neighbor in H_i . Construct a graph G' from G by contracting H_1, \dots, H_k into v_1, \dots, v_k , respectively. If G admits a 2-stable trace W then G' admits a 2-stable trace W' , which traverses edges from $E(G) \cap E(G')$ in the same direction as W .*

Proof. Suppose that a graph G admits a 2-stable trace W . We proceed by induction on the number k of pairwise edge and vertex disjoint subtrees required to be contracted in G in order to construct G' . If $k = 0$ then $G' = G$ and therefore W is a 2-stable trace in G' .

Let $k \geq 1$ and let G_1 be a graph that we get if we contract H_1 into v_1 in G . Construct a double trace W_1 from W as follows. We start in an arbitrary vertex of $V(G) \setminus V(H_1)$ and follow W . Let $a = xy$ be an arc of W that we are currently traversing on our walk along W . If $x, y \in V(G) \setminus V(H_1)$, then we put xy into W' so that the order of arcs from W is preserved. If $x \in V(H_1)$ and $y \notin V(H_1)$ then we put v_1y in W_1 instead of a . Similarly, we replace arcs where $x \notin V(H_1)$ and $y \in V(H_1)$ with xv_1 . Finally, the occurrences of the arcs from H_1 are ignored in W_1 .

We claim that W_1 is a 2-stable trace of G_1 . Since every edge is traversed twice in W , every edge is traversed twice in W_1 . Hence W_1 is a double trace. If W_1 is not a 2-stable trace, there exists a vertex $x \in V(G_1)$ such that W_1 has an 1-repetition or a 2-repetition at x . Denote the neighborhood of vertex v_1 in G_1 with $N(v_1)$. We have to consider three cases.

Case 1: $x \notin N(v_1)$.

It is clear from the construction that if W_1 had an 1-repetition or a 2-repetition at x , already W would have an 1-repetition or a 2-repetition at x , a contradiction.

Case 2: $x \in N(v_1)$.

It is again clear from the construction that if W_1 had an 1-repetition xyx or a 2-repetition xyz , where $y, z \neq v_1$, already W would have an 1-repetition or a 2-repetition at x , a contradiction.

Assume first that W_1 has an 1-repetition v_1xv_1 . It follows that W should contain hgx , where $h, g \in H_1$. Since every vertex in $V(G) \setminus V(H_1)$ has at most one neighbor in H_1 , $h = g$. Therefore W should contain an 1-repetition hxx , a contradiction.

Assume next that W_1 has a 2-repetition v_1xy for some neighbor y of x . It follows that W should contain hxy and gxy , where $h, g \in H_1$. Since every vertex in $V(G) \setminus V(H_1)$ has at most one neighbor in H_1 , $h = g$. Therefore W should contain a 2-repetition hxy , a contradiction.

Case 3: $x = v_1$.

Assume first that W_1 has an 1-repetition yv_1y for some neighbor y of v_1 . It follows that W should contain $yhAhy$, where h is a unique neighbor of y in H_1 and A is a circuit in H_1 . Since H_1 is a tree, the only possibility that circuit appears in a part of a double trace W that is completely included in H_1 is with an 1-repetition, a contradiction.

Assume next that W_1 has a 2-repetition yv_1z for some neighbors y and z of v_1 . It follows that W should contain $yhBgz$ and $yhCgz$, where h is a unique neighbor of y in H_1 , g is a unique neighbor of z in H_1 , while B and C are hg -paths in H_1 . If $h = g$, similarly as before follows that W should have an 1-repetition. Otherwise, if $h \neq g$, we

can use the fact that in a tree any two vertices are connected with unique path to argue that $B = C$ and therefore that already W should have a 2-repetition, a contradiction.

We have thus proved that W_1 is a 2-stable trace in G_1 . During the construction of W_1 we did not change the direction of any arc from W . Since G' can be constructed from G_1 by contracting the remaining $k - 1$ pairwise edge and vertex disjoint subtrees H_2, \dots, H_k into v_2, \dots, v_k , respectively, it follows by the induction assumption that G' admits a 2-stable trace (which traverses edges from $E(G) \cap E(G')$ in the same direction as W). \square

The following was proven in [6], where it was also observed that a graph G admits a parallel double trace if and only if G is Eulerian.

Proposition 2.2 [6, Proposition 5.4] *A connected graph G admits a parallel 1-stable trace if and only if G is Eulerian.*

Proof. Traverse an arbitrary Eulerian circuit of graph G twice in the same direction to obtain a parallel 1-stable trace. \square

We next prove Theorem 2.3 about parallel 2-stable traces and then use it in Section 3 to present an alternative proof of Theorem 3.1.

Theorem 2.3 *A graph G admits a parallel 2-stable trace if and only if G is Eulerian and $\delta(G) > 2$.*

Note that for Eulerian graphs a constraint on the minimal degree of a graph from Theorem 2.3 is equivalent to $\delta(G) \geq 4$.

Proof. Suppose that a graph G admits a parallel 2-stable trace. By definition, every 2-stable trace is an 1-stable trace. Thus by Proposition 2.2, G is Eulerian and hence by Proposition 1.1 we infer that $\delta(G) \geq 4$.

For the converse assume that G fulfills the conditions of the theorem. We proceed by induction on $\Delta = \Delta(G)$.

Let $\Delta = 4$. Then $\delta(G) = \Delta(G) = 4$. By Proposition 2.2, G admits a parallel 1-stable trace W' . If W' is not already a 2-stable trace, W' contains at least one 2-repetition. We proceed with the second induction on the number k of vertices where W' has 2-repetitions. Let $k \geq 1$ and let v be one of the vertices where W' has a 2-repetition. If an 1-stable trace W' has a 2-repetition through v , where v is a vertex with $d_G(v) = 4$, then it is not difficult to see that W' has two 2-repetitions through v . Let v_1, v_2, v_3 , and v_4 be the neighbors of v . Without loss of generality, we can assume that $A = v_1 \rightarrow v \rightarrow v_2$ is the first and $B = v_3 \rightarrow v \rightarrow v_4$ is the second 2-repetition through v in W' . That means that sequences A and B appear twice in W' . Because W' is a parallel 1-stable trace, there are only two possibilities how occurrences of A and

B are arranged in W' . These possibilities are $AABB$ (Fig. 3, left) and $ABAB$ (Fig. 4, left). Note that we left out all the other vertices in Figs. 3 and 4.

In the first case we construct a double trace W from W' in G as follows. We start in an arbitrary vertex of $V(G) \setminus \{v\}$ and follow W' . Let $a = xy$ be an arc of W' that we are currently traversing on our walk along W' . If $x, y \in V(G) \setminus \{v, v_1, v_2, v_3, v_4\}$, then we put xy into W so that the order of arcs from W' is preserved. Put one occurrence of $v_1 \rightarrow v \rightarrow v_2$ and one occurrence of $v_3 \rightarrow v \rightarrow v_4$ in W as well. Replace the remaining occurrence of $v_1 \rightarrow v \rightarrow v_2$ with $v_1 \rightarrow v \rightarrow v_4$ and the remaining occurrence of $v_3 \rightarrow v \rightarrow v_4$ with $v_3 \rightarrow v \rightarrow v_2$, such that W stays connected, see Fig. 3, right.

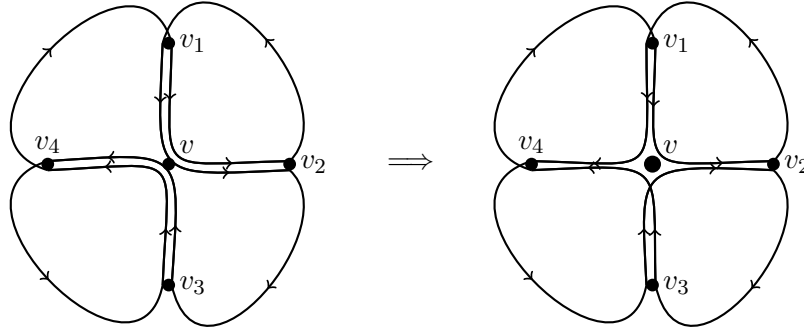


Figure 3: Removing 2-repetition through v (case $AABB$)

We construct W analogously in the second case, see Fig. 4, right.

We claim that in both cases W is a parallel 1-stable trace of G with at least one vertex with 2-repetition less than W' . Note first that any edge $e = xy$ that appears in W (arcs xy or yx appears in W) has its unique corresponding edge e' in W' . Any edge $e = xy$ in W , where $x \neq v$ and $y \neq v$, is traversed twice in the same direction in W because it is traversed twice in the same direction in W' . Four remaining edges (vv_1 , vv_2 , vv_3 , and vv_4) are traversed twice in the same direction by construction. Hence W is a parallel double trace. It is also clear from the construction that W is an 1-stable trace. Finally we need to verify that W has at least one vertex with 2-repetition less than W' . Let x be an arbitrary vertex of G in which W has a 2-repetition. We have to consider three cases.

Case 1: $x \notin \{v, v_1, v_2, v_3, v_4\}$.

It is clear from the construction that if W has a 2-repetition through x , also W' has a 2-repetition through x .

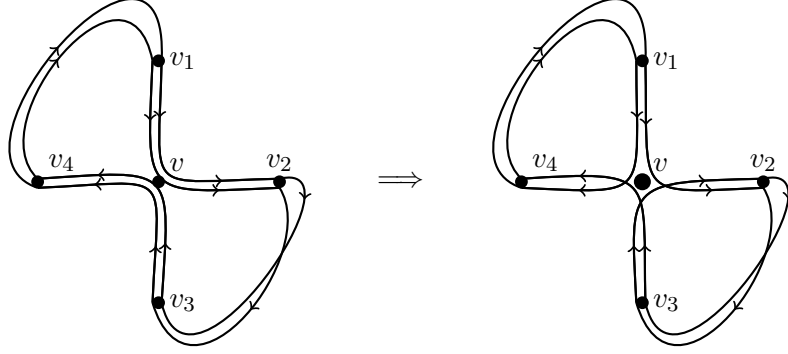


Figure 4: Removing 2-repetition through v (case $ABAB$)

Case 2: $x \in \{v_1, v_2, v_3, v_4\}$.

It is again clear from the construction that if W has a 2-repetition yxz , where $y, z \neq v$, also W' has a 2-repetition through x .

Similarly, if W has a 2-repetition vxy for some neighbor y of x , also W' has a 2-repetition through x since the order of arcs adjacent to $\{v_1, v_2, v_3, v_4\}$ did not change in W .

Case 3: $x = v$.

1-stable trace W' had a 2-repetition (two 2-repetitions to be more accurate) through v but during the construction of W we manage to remove them both.

We have thus constructed an 1-stable trace W which have at least one vertex with 2-repetition less than W' . Hence, it follows by induction assumption that any 4-regular graph admits a parallel 2-stable trace.

Assume now that $\Delta \geq 6$ and that any graph H with $\Delta(H) < \Delta$ which fulfills the conditions of Theorem 2.3 admits a parallel 2-stable trace. We have to again consider two cases.

Case 1: $\Delta \equiv 2 \pmod{4}$.

Construct the graph G' from G as follows. For every vertex v of degree Δ (temporary denote its neighbors with v_1, \dots, v_Δ) repeat next procedure. Remove v from G . Add two new vertices v' and v'' , connect them by an edge, connect v' with $v_1, \dots, v_{\frac{\Delta}{2}}$, and connect v'' with the remaining neighbors of v , see Fig. 5.

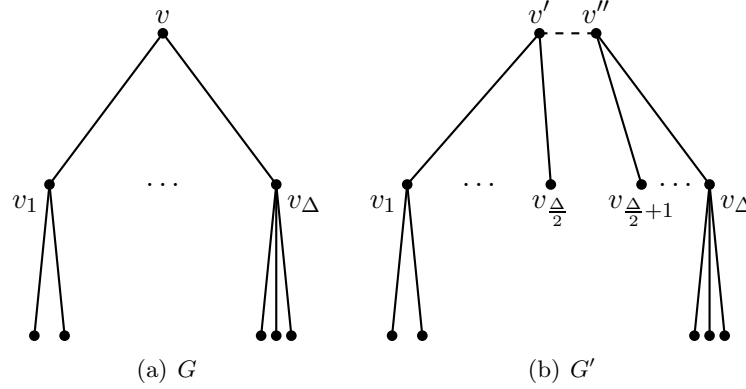


Figure 5: Construction from the proof of Theorem 2.3 for the case $\Delta \equiv 2 \pmod{4}$

Note that in G' all except the newly added vertices are of the same degree as in G , while $d_{G'}(v') = \frac{\Delta}{2} + 1$ and $d_{G'}(v'') = \frac{\Delta}{2} + 1$ (the last two statement are true for all new vertices). It follows that $\Delta(G') < \Delta$. Since $\Delta \geq 6$, we also infer that $\delta(G') \geq 4$. Because $\Delta \equiv 2 \pmod{4}$, the degrees $d_{G'}(v') = d_{G'}(v'') = \frac{\Delta}{2} + 1$ are even, hence G is Eulerian and by the induction assumption on Δ , G' admits a parallel 2-stable trace. It follows from Lemma 2.1 that G admits a parallel 2-stable trace.

Case 2: $\Delta \equiv 0 \pmod{4}$.

Construct the graph G' from G as follows. For every vertex v of degree Δ (temporary denote its neighbors with v_1, \dots, v_Δ) repeat next procedure. Remove v from G , and add three new vertices v' , v'' , and v''' . Connect v'' with v' and v''' by an edge, connect v' with $v_1, \dots, v_{\frac{\Delta}{2}-1}$, connect v'' with $v_{\frac{\Delta}{2}}$ and $v_{\frac{\Delta}{2}+1}$, and connect v''' with the remaining neighbors of v , see Fig. 6.

Analogously as in the first case, note that in G' all except the newly added vertices are of the same degree as in G , while $d_{G'}(v') = d_{G'}(v''') = \frac{\Delta}{2}$ and $d_{G'}(v'') = 4$ (the last two statement are true for all new vertices). It follows that $\Delta(G') < \Delta$. Since $\Delta \geq 6$, we also infer that $\delta(G') \geq 4$. Because $\Delta \equiv 0 \pmod{4}$, the degrees $d_{G'}(v') = d_{G'}(v''') = \frac{\Delta}{2}$ are even, hence G is Eulerian. By the induction assumption on Δ , G' admits a parallel 2-stable trace. It follows from Lemma 2.1 that G admits a parallel 2-stable trace.

We have thus proved Theorem 2.3. \square

3 Parallel d -stable traces

We now use results from previous section to present an alternative proof of next theorem from [2].

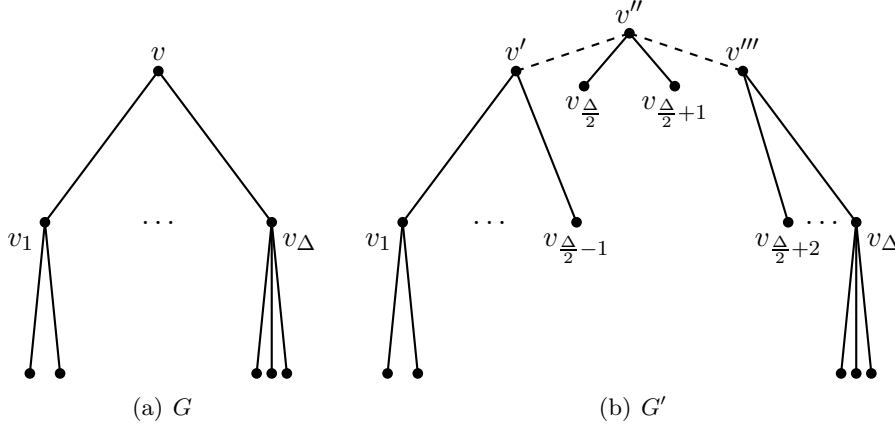


Figure 6: Construction from the proof of Theorem 2.3 for the case $\Delta \equiv 0 \pmod{4}$

Theorem 3.1 [2, Theorem 5.4] *A graph G admits a parallel d -stable trace if and only if G is Eulerian and $\delta(G) > d$.*

Proof. From Proposition 1.1 it follows that for every graph G , which admits a d -stable trace, $\delta(G) > d$. Since every edge of a parallel double trace is used twice in the same direction, input and output degree of a parallel double trace W would not match at the vertex of odd degree, which is absurd.

For the converse assume that graph G is Eulerian and $\delta(G) > d$. We can also assume that $\delta(G)$ is an even number. Furthermore, since for parallel 1-stable traces and 2-stable traces theorem follows from Proposition 2.2 and Theorem 2.3, respectively, we can assume that $d \geq 3$. Denote a graph obtained from G by replacing every vertex v of degree $d_G(v) > 4$ with $(d_G(v) - 2)/2$ new vertices, connected into a path P_v , as describe in the proof of Theorem 2.3, with G' . Additionally, connect two endvertices of P_v with three different neighbors of v and each inner vertex of P_v with two different remaining neighbors, so that each of the vertices from $N(v)$ is connected to exactly one vertex in P_v . It is not difficult to see that G' is a 4-regular graph and therefore by Theorem 2.3 admits a parallel 2-stable trace W' . Construct a parallel double trace W in G from W' as follows. We start in an arbitrary vertex of G' and follow W' . Let $a' = xy$ be an arc of W' that we are currently traversing on our walk along W' . If for every v , $d_G(v) > 4$, $x, y \notin V(P_v)$, then we put xy into W so that the order of arcs from W' is preserved. If for some v , $d_G(v) > 4$, $x \in P_v$ or $y \in P_v$, we replace a' with vy or xv , respectively. Finally, occurrences of the arcs with both endvertices contained in some P_v are ignored in W .

We claim that a parallel double trace W is a parallel d -stable trace of graph G . We assume conversely and denote an arbitrary vertex in which W has a repetition of order $\leq d$ with v . Denote the maximal order of $(\leq d)$ -repetition at v with d' . Since

we used the same construction as in the proof of Theorem 2.3, it follows that W is a parallel 2-stable trace (and $d' > 2$). From the symmetry of repetitions it also follows that $d_G(v) > d' + 2$, since otherwise W would have at least one 1-repetition or one 2-repetition at v (therefore also $d_G(v) \geq 8$). It is also not difficult to see that every repetition in a parallel double trace is of even degree. Denote the subset of $N(v)$, containing vertices from maximal repetition at v , with N ($|N| = d'$). There exists a path P_v in G' that during the construction replaced v from G . To make the argument more transparent, we imagine vertices from P_v arranged in a horizontal line with all the neighbors of v from $N(v)$ except for two, lying directly above or below vertices of P_v . The remaining two neighbors of vertex v are aligned at the beginning and at the end of the horizontal line containing vertices from P_v . Fig. 7 (b) shows P_v with vertices from $N(v)$ in G' for $d_G(v) = 8$ (v' , v'' , and v''' are the vertices replacing v in G'). Next, we color vertices from $N(v)$ with two colors—black and white, such that vertices from N are colored black while vertices from $N(v) \setminus N$ are colored white. Example of such coloring can be seen at Fig. 7.

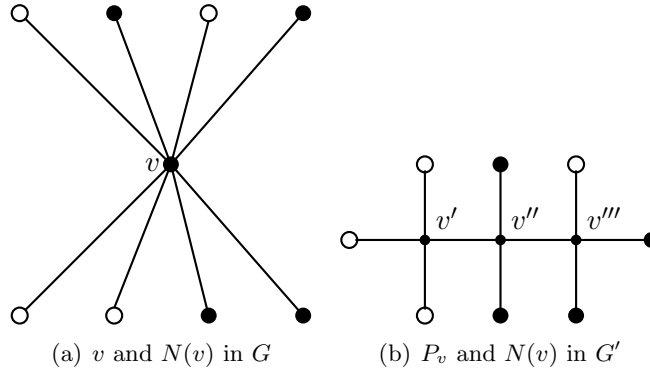


Figure 7: Structures of $N(v)$ in G and P_v in G' . Vertices contained in N are colored black.

Since the subset $N(v) \setminus N$ is also a repetition, the arguments used hereinafter are true for black and white vertices and we can, without loss of generality, assume that the neighbor of $N(v)$, lying farthest to the left in the above mentioned horizontal line is colored white. We next move along this horizontal line and denote the first black vertex that we met (below or above the line) with b . Denote its neighbor in P_v with v' . Since there are at least four black vertices, v' is not the farthest right vertex from P_v . Therefore, we can also denote the right neighbor of v' from P_v with v'' and consider two cases. In the first case b is the only neighbor of v' ($\notin P_v$) colored black (Fig. 8 (a)), while in the second case also the second neighbor of v' ($\notin P_v$) is colored black (Fig. 8 (b)). In both cases we can, without loss of generality, assume that an edge bv' is traversed twice in the direction toward v' in W' (arc bv' is traversed twice in W ,

while arc $v'b$ does not appear in W'). It follows from the fact that a subset $N \subseteq N(v)$ is an N -repetition of W , that every time a double trace W comes to v from a vertex in N it also continues to a vertex in N and, consequently, that every time a double trace W' comes to a vertex in P_v from a (black colored) vertex in N it also leaves to a (black colored) vertex in N . Note that in between W' can traverse other vertices from P_v . Analogously is true for (white colored) vertices from $N(v) \setminus N$. Therefore, two subsequences which start with bv' , continue on some other vertices from P_v and end in two from b different vertices from N , exist in W' . In the first case, when b is the only black colored neighbor of v' , $b \rightarrow v' \rightarrow v''$ has to appear twice in W' , since otherwise W' can not continue (twice) from b to a black colored vertices without previously traversing white vertex. This contradicts the fact that W' is a parallel 2-stable trace, since $bv'v''$ is a 2-repetition at v' . In the second case, we denote l (l is an odd integer) white vertices that appear to the left of b with w_1, \dots, w_l . For example see Fig. 8 (b), where those vertices are denoted with w_1, w_2 , and w_3 . Next, we denote the second black colored neighbor of v' from $N(v)$ with b' . Since subsequence $b \rightarrow v' \rightarrow b'$ can appear at most once in W' (otherwise W' would have a 2-repetition at v') and since for at least one of the vertices w_1, \dots, w_l , W' has to continue to a white colored vertex different from w_1, \dots, w_l (otherwise vertices w_1, \dots, w_l would form an odd repetition in W , which can not appear in a parallel 2-stable trace), it follows that an edge $v'v''$ (arc $v'v''$ and $v''v'$) are used more than twice in W' , which is absurd.

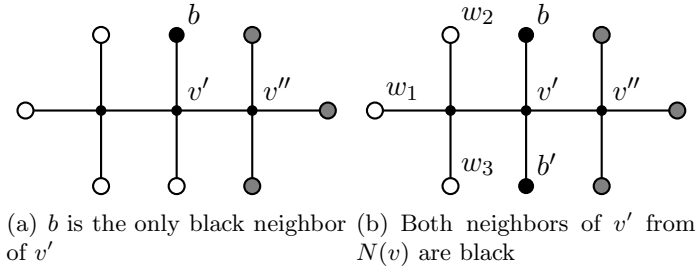


Figure 8: Two cases of the structure of P_v (of v' and b to be more precise). Vertices for which the color is not determined are colored grey.

Since v was an arbitrary vertex in G and d' was an arbitrary integer, $2 < d' \leq d$, it follows that W is a parallel d -stable trace of G and therefore Theorem 3.1 is proved. \square

4 Concluding remarks

In this section we present two concepts for which we assumed that could be used for constructing parallel 2-stable traces. Unfortunately, it has turned out, when proving

Theorem 2.3, that there exists graphs admitting only parallel 2-stable traces which can not be realized using here described constructions.

The first construction goes as follows. Let G be an Eulerian graph with n vertices (denoted with v_1, \dots, v_n) fulfilling conditions of Theorem 2.3 and let W' be an Eulerian circuit of G . W' induces a set of functions $\Pi' = \{\pi'_1, \dots, \pi'_n\}$, where $\pi'_i : V(G) \setminus \{v_i\} \rightarrow V(G) \setminus \{v_i\}$, $\pi'_i(v) = u$ if and only if $v \rightarrow v_i \rightarrow u$ is a sequence in W' , for $1 \leq i \leq n$. Note that $u \neq v$, because G is simple and W' traverses every edge exactly once. Construct another Eulerian circuit W'' in G such that it will induce a set of functions $\Pi'' = \{\pi''_1, \dots, \pi''_n\}$ with above described characteristics. In addition demand, that edges are traversed in the same direction as in W' , and that if $\pi'_i(v) = u$ then $\pi''_i(v) \neq u$ and $\pi''_i(u) \neq v$. The last already follows from the fact that all the edges are traversed twice in the same direction as in W' . Concatenate Eulerian circuits W' and W'' into a double trace W in an arbitrary vertex v . Be careful that this does not rise any 1-repetition or 2-repetition in v . It is obvious from the construction that every edge is traversed twice in the same direction in W and that W is without 1-repetitions and 2-repetitions in any other vertex than v . Hence, if a graph G admits two Eulerian circuits with above described characteristic, G admits parallel 2-stable trace as well.

It turns out that, we cannot always construct a parallel 2-stable trace of G by concatenating two Eulerian circuits. For instance, the graph G from Fig. 9 has a parallel 2-stable trace: $v_1 \rightarrow v_2 \rightarrow v_3 \rightarrow v_1 \rightarrow v_2 \rightarrow v_4 \rightarrow v_1 \rightarrow v_5 \rightarrow v_2 \rightarrow v_3 \rightarrow v_4 \rightarrow v_6 \rightarrow v_5 \rightarrow v_2 \rightarrow v_4 \rightarrow v_6 \rightarrow v_7 \rightarrow v_9 \rightarrow v_8 \rightarrow v_6 \rightarrow v_7 \rightarrow v_{10} \rightarrow v_8 \rightarrow v_{11} \rightarrow v_7 \rightarrow v_9 \rightarrow v_{10} \rightarrow v_{11} \rightarrow v_7 \rightarrow v_{10} \rightarrow v_{11} \rightarrow v_9 \rightarrow v_8 \rightarrow v_{11} \rightarrow v_9 \rightarrow v_{10} \rightarrow v_8 \rightarrow v_6 \rightarrow v_5 \rightarrow v_3 \rightarrow v_1 \rightarrow v_5 \rightarrow v_3 \rightarrow v_4 \rightarrow v_1$, but because of the cut vertex v_6 , from any Eulerian circuit W of G we cannot construct another Eulerian circuit with the described properties.

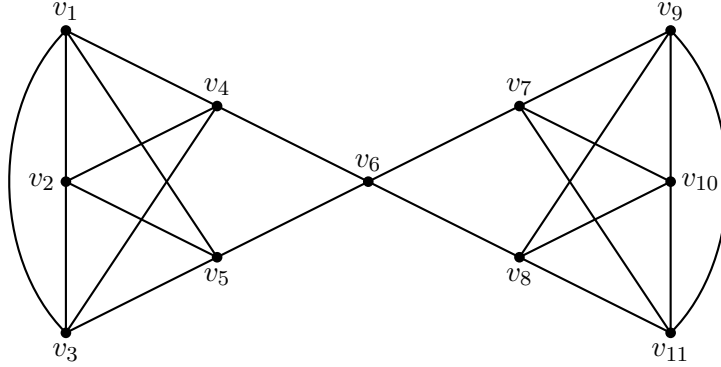


Figure 9: Graph whose parallel 2-stable traces cannot be constructed by concatenating two Eulerian circuits

The main idea of the second construction is to find a parallel 2-stable trace in each block of graph G and then concatenate them into a parallel 2-stable trace of graph

G . Let again G be an Eulerian graph fulfilling the conditions of Theorem 2.3. Denote blocks of G with B_1, \dots, B_k and cutvertices with v_1, \dots, v_l . Find first a parallel 2-stable trace W_i in block B_i . Concatenate parallel 2-stable traces into a parallel 2-stable trace of G in corresponding cutvertices. When concatenating, one has to be careful that no 1-repetitions and 2-repetitions appear.

Similar as for the first construction, none of the parallel 2-stable traces of graph G from Fig. 9 can not be constructed by concatenating parallel 2-stable traces in its blocks. Vertex v_6 is a unique cutvertex of graph G and it is contained in both of its blocks. Since v_6 is of degree 2 in both blocks of graph G , none of them admit parallel 2-stable trace. Similar problem occurs if one or more blocks of G are bridges.

We could instead of parallel 2-stable traces in blocks demand parallel 1-stable traces where 2-repetitions (or 1-repetitions if block is a bridge) are allowed at cutvertices but are later removed during the concatenation into a parallel 2-stable trace of the whole graph. Even this modification does not give us an algorithm for constructing a parallel 2-stable trace in an arbitrary graph. By Theorem 2.3 the graph G from Fig. 10 has a parallel 2-stable trace. However, two of its block have vertices of degree 3 (v_1, v_2, v_3 , and v_4) and therefore by Proposition 2.2 do not admit neither parallel 1-stable trace nor parallel 2-stable trace.

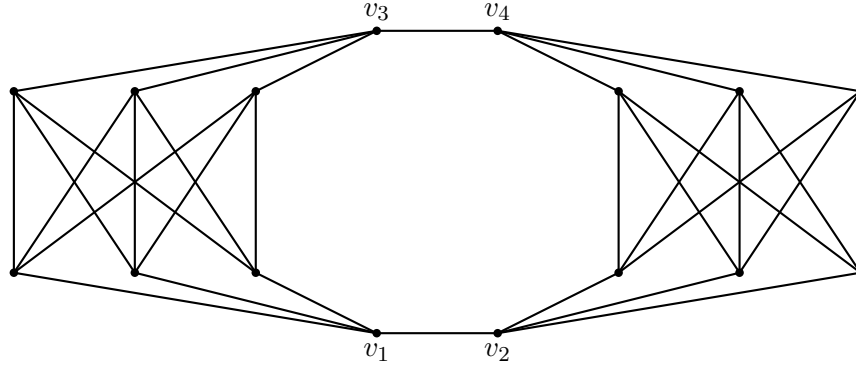


Figure 10: Graph whose parallel 2-stable trace cannot be constructed by concatenating parallel 1-stable or parallel 2-stable traces in blocks of a graph

Acknowledgements

The author is grateful to Sandi Klavžar and anonymous reviewers for several significant remarks and suggestions which were of great help. The research was in part financed by Slovenian Research Agency under the grants P1-0297 and L7-5554.

References

- [1] R.B. Eggleton, D.K. Skilton, *Double tracings of graphs*, Ars Combin. **17A** (1984), 307–323.
- [2] G. Fijavž, T. Pisanski, and J. Rus, *Strong traces model of self-assembly polypeptide structures*, MATCH Commun. Math. Comput. Chem. **71** (2014), 199–212.
- [3] H. Fleischner, Eulerian Graphs and Related Topics. Part 1. Vol. 2., North-Holland, Amsterdam, 1991.
- [4] H. Gradišar, S. Božič, T. Doles, D. Vengust, I. Hafner Bratkovič, A. Mertelj, B. Webb, A. Šali, S. Klavžar, R. Jerala, *Design of a single-chain polypeptide tetrahedron assembled from coiled-coil segments*, Nature Chem. Bio. **9** (2013), 362–366.
- [5] H. Gradišar, R. Jerala, *De novo design of orthogonal peptide pairs forming parallel coiled-coil heterodimers*, J. Peptide Sci. **17** (2011), 100–106.
- [6] S. Klavžar, J. Rus, *Stable traces as a model for self-assembly of polypeptide nanoscale polyhedrons*, MATCH Commun. Math. Comput. Chem. **70** (2013), 317–330.
- [7] G. Sabidussi, *Tracing graphs without backtracking*, Operations Research Verfahren XXV, Symp. Heidelberg, Teil **1** (1977), 314–332.
- [8] J. Rus, *Antiparallel d-stable traces and a stronger version of Ore problem*, J. Math. Biol. (2016), to appear, DOI: 10.1007/s00285-016-1077-2.
- [9] D. B. West, Introduction to Graph Theory, Prentice Hall, Upper Saddle River, 1996.